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PB-282 885

Time Series Experiments for Studying Plant Growth Response to Pollution

Corvallis Environmental Research Lab, Oreg.

Apr 78

EPA-600/3-78-038
April 1978

PB 282 885

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TECHNICAL REPORT DATA
(Please read Instructions on the reverse before completing)

1. REPORT NO. EPA-600/3-78-038	2.	3. RECIPIENT'S ACCESSION NO. PB282885
4. TITLE AND SUBTITLE "Time Series Experiments for Studying Plant Growth Response to Pollution"		5. REPORT DATE April 1978 6. PERFORMING ORGANIZATION CODE
7. AUTHOR(S) Larry Male, John Van Sickle, and Ray Wilhour		8. PERFORMING ORGANIZATION REPORT NO.
9. PERFORMING ORGANIZATION NAME AND ADDRESS Assessment & Criteria Development Division Ecosystems Modeling & Analysis Branch Corvallis Environmental Research Laboratory 200 S.W. 35th St. -- Corvallis, OR 97330		10. PROGRAM ELEMENT NO. 1AA602 11. CONTRACT/GRANT NO.
12. SPONSORING AGENCY NAME AND ADDRESS U.S. Environmental Protection Agency - Corvallis, OR Corvallis Environmental Research Center 200 S.W. 35th St. Corvallis, OR 97330		13. TYPE OF REPORT AND PERIOD COVERED Inhouse 14. SPONSORING AGENCY CODE EPA/600/02
15. SUPPLEMENTARY NOTES		

16. ABSTRACT

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This report covers a period from April 1974 to September 1977 and was completed as of February 1978.

17. KEY WORDS AND DOCUMENT ANALYSIS

a. DESCRIPTORS	b. IDENTIFIERS/OPEN ENDED TERMS	c. COSATI Field/Group
Sulfur Dioxide Time Series Analysis Experimental Design		Field 06/F 06/S

18. DISTRIBUTION STATEMENT Release Unlimited	19. SECURITY CLASS *(This Report)* UNCLASSIFIED 20. SECURITY CLASS *(This page)* UNCLASSIFIED	21. NO. OF PAGES 26 22. PRICE PC A03/MF A01

EPA Form 2220-1 (Rev. 4-77) PREVIOUS EDITION IS OBSOLETE

* U.S. GOVERNMENT PRINTING OFFICE: 1978—796-747/139 REGION 10

EPA-600/3-78-038
April 1978

TIME SERIES EXPERIMENTS FOR STUDYING PLANT GROWTH RESPONSE TO POLLUTION

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FOREWORD

Effective regulatory and enforcement actions by the Environmental Protection Agency would be virtually impossible without sound scientific data on pollutants and their impact on environmental stability and human health. Responsibility for building this data base has been assigned to EPA's Office of Research and Development and its 15 major field installations, one of which is the Corvallis Environmental Research Laboratory (CERL).

The primary mission of the Corvallis Laboratory is research on the effects of environmental pollutants on terrestrial, freshwater, and marine ecosystems; the behavior, effects and control of pollutants in lake systems; and the development of predictive models on the movement of pollutants in the biosphere.

This report details research aimed at establishing functional relationships between agricultural crop losses and natural variations in SO_2 air pollution.

A.F. Bartsch
Director, CERL

ABSTRACT

This research program was initiated with the overall objective of defining experiments which could predict the yield losses of crops grown under naturally varying sulfur dioxide concentrations.

A model for simulating realistic fluctuations in SO_2 air pollution was developed. This model was used to design experiments in field growth chambers for the purpose of establishing the functional and probabilistic relationship between yield loss and median SO_2 concentration. The stochastic experiments are offered as a viable alternative to traditional long-term fixed concentration experiments.

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SECTION 1

INTRODUCTION

A fundamental problem in air pollution-plant effects research is to predict the reduction in yield of crops grown in areas of significant SO_2 stress. Within such areas the pollutant concentration at any point in time is only probabilistically predictable, i.e., we can only predict the probability that the concentration will fall within a specified interval. Assuming the SO_2 source strength in an area does not vary over time, then the fluctuations in pollutant concentration are caused primarily by random variations in wind speed. The time history of pollutant concentrations within an area is called a time series. Pollutant time series for different growing seasons will appear to be considerable different but they will usually be probabilistically the same. Because of this probabilistical regularity, a model with a maximum of two or three parameters can simulate certain pollutant time series. It is our purpose in this paper to motivate the use of a time series model for experimentally studying the long term effect on plant growth of stochastically (probabilistically) varying pollutant concentrations.

As a first step we might ask "What relationship might we expect between crop yield and a pollutant time series?" We hypothesize that plant growth rate will fluctuate in correspondence with the pollutant time series? Assume for the moment that growth rate is depressed by the pollutant. Plant yield would then be the integral, over the growing season, of the resulting growth rate time series. Since pollutant time series within different growing seasons are probabilistically the same, we would expect growth rate time series to be probabilistically the same. Hence we would expect yield in different growing seasons to be probabilistically the same. Ideally, knowledge of the pollutant probability distribution would allow one to predict, for any growing season, the probability that yield would be within any specified range.

The above model assumes that there is a simple relationship between instantaneous growth rate and pollutant concentration, but establishing this relationship is not trivial. It is not practical to continuously monitor growth rate in order to study its relationship with randomly varying pollutant concentration. Even if it were possible to monitor growth rate it would be an exceedingly complex task to correlate it with observed fluctuations in

pollutant concentration. In order to achieve a desirable precision, a model would have to consider response time lags, recovery rate at different concentrations, adaptation, and of course variation in other environmental variables which affect growth rate. Such a model may eventually prove to be our best predictive tool but we must wait for further technological development.

If we cannot construct a model which will predict growth rate as a function of pollutant concentration and other environmental variables then we might ask whether there exists a single summary statistic for a pollutant time series which would correlate well with plant yield. We cannot answer this question here, but we can suggest an experimental approach which can be used to define the relationship between long term growth response and summary statistics for a pollutant time series.

One experimental technique which has been used to estimate the effect of SO_2 on crop yield is the "long-term fixed concentration experiment." Plants are subjected to a fixed SO_2 concentration for an entire growing season. A variation of this experiment is the use of intermittent exposures (say, exposure every other week). The critical assumption underlying this approach is that reductions in yield would be the same as if the pollutant concentration had varied stochastically about an average equal to the experimentally fixed concentration. Since this type of experiment violates our hypotheses concerning the interactions of growth rate and pollutant concentration we suggest abandoning it in favor of experiments which expose plants to a realistic pollutant concentration schedule over the entire growing season at near-ambient environmental conditions. The final yield of the plants would then be correlated with summary statistics which characterize the entire pollutant regime to which the plants were exposed.

This strategy has led to at least three different experimental methods which appear promising. Oshima et al. (1976) conducted growth experiments based on environmental gradient analysis. In this design, crops are grown in identical field plots maintained at different distances from a strong urban oxidant source, thus providing a natural gradient in average concentration and dose. A second method is the zonal air pollution system (ZAPS), described by Lee et al. (1975). The system employs grids of pipes that dispense gaseous pollutants on field plots. Source strength is varied over several plots to create a gradient of average concentrations, and local variations in wind speed produce realistic short-term fluctuations in concentration.

A third approach, described here, uses closed field chambers to control the SO_2 regime. Pollutant concentrations in the chambers are changed hourly, thus plants are exposed to an arbitrary, rapidly changing time series of pollutant concentrations. This flexibility provides a distinct advantage over the natural gradient and ZAPS methods which depend on local meteorological conditions for concentration variability.

These approaches are sensible only if one can quantitatively summarize long, continuously-changing time series of pollutant concentrations. Fortunately, traditional statistical analyses (Larsen, 1971) coupled with advances in time series analysis techniques (Box and Jenkins, 1976; Jenkins and Watts, 1968) have begun to satisfy this need.

When experimental pollutant concentrations are controlled on an hour-by-hour basis, as in the closed field chambers, one must also be able to reproduce realistic time series of pollutants. This paper describes models which will generate such time series and discusses the design of plant growth studies based on the models.

The following section is a brief, qualitative description of the pollutant time series observed in the ambient environment.

The final sections provide mathematical descriptions of observed time series and present models which simulate those observations. We also discuss experimental design problems which arise when the models are used to generate pollutant exposure schedules.

SECTION 2

GENERAL CHARACTERISTICS OF OBSERVED POLLUTANT LEVELS

The standard method of summarizing concentration levels observed over a long time interval is to plot their relative frequencies of occurrence. Typically the data consist of low concentrations with infrequent occurrences of high concentrations. Thus, the frequency curves can usually be described by a lognormal distribution, over a broad range of pollutant types and source configurations (Larsen, 1971; Lee et al. 1975; Gifford, 1974; and Bencala and Seinfeld, 1976). Gifford (1974) and Knox and Pollack (1974) provide a simple theoretical explanation of the observed lognormality. They argue that a pollutant from several sources, as seen in urban areas, tends to have concentration levels which are highly correlated over short time intervals, and they show how this leads to a lognormal frequency curve.

If concentrations are distributed lognormally, they can be summarized by a median and shape parameter as described in Section 3. In assessing the variable response of vegetation to ambient pollution concentration distributions, it is sufficient to correlate plant response with two parameters of the distribution, the median concentration and the shape parameter.

A common test for lognormality is to see whether the empirical distribution function plots as a straight line on logarithmic-probability paper. The Air Quality Criteria for Sulfur Oxides (1970) shows the empirical distribution functions for SO_2 concentration for six large cities across the United States (Continuous Air Monitoring Project [CAMP], 1962-1967, one-hour averaging time). These distributions, plotted on logarithmic-probability paper, range from slightly curved to approximately straight lines. A general impression is that they could be approximately modeled as a family of parallel straight lines. This is equivalent to saying that the concentrations are lognormally distributed with a common shape parameter but with varying medians.

A possible explanation for this phenomenon is that the shape parameter is determined by meteorological factors independently of source strength of the pollutant while the median is determined primarily by source strength. This explanation is supported empirically by studies with the Zonal Air Pollution Study (Lee et al., 1975).

Another set of characteristics emerges when pollutant concentrations are considered as a time series. They have regular fluctuations which can often be correlated with human activity patterns (i.e., source strength) as well as periodic weather variables (Raynor et al., 1974; Holzworth, 1973; Munn and Katz, 1959). Most concentration time series show 24-hour cycles, but the timing and shape of the diurnal patterns depend upon pollutant type, geographic location, and season. Yearly cycles as well usually appear in pollution data, but for most cases the changes are too slow to be observed over the length of a growing season.

Concentration series are also highly correlated over short time intervals. Often one can assume the time series is stationary over a growing season--that is, the median and shape parameter of the concentration distribution stay constant. In this case, the degree of serial correlation, or autocorrelation, exhibited by a series can usually be specified by one parameter. The parameters can be correlated to the response of plants when they are exposed to rapidly fluctuating pollutant levels (low autocorrelation) as opposed to slowly-changing levels (high autocorrelation).

These observations provide a basis for simple dynamic models of pollutant concentrations. The models are used to generate exposure schedules for plant growth experiments in closed field exposure chambers. Several models of different degrees of realism and complexity are being explored in an attempt to identify those features of long-term, continuously-varying pollutant concentrations to which plants are most sensitive. The following sections describe observed concentration time series in more detail and present the models used.

SECTION 3

EXPERIMENTAL TIME SERIES MODELS

To perform a controlled time series experiment, a model must be used to generate exposure schedules. Varying levels of realism can be incorporated into this model by making it more or less complex. The first step in constructing the model is to decide what features of a natural time series are important for simulation. We will first deal with stochastic time series.

STATIONARY STOCHASTIC MODELS

In the previous section we summarized the properties of a natural pollutant time series. We must now model these properties with a set of mathematical assumptions. The criteria that we feel are important for a pollutant time series model are:

(1) Lognormally distributed concentrations.

(2) Stationarity, i.e., the distribution of concentration is time invariant.

(3) Autoregressive, i.e., future concentrations depend upon past behavior.

(4) Realistic autocorrelation function, i.e., similar to the natural time series reported in Pollack, 1973, and Barlow and Singpurwalla, 1974.

In particular, we will assume that the concentration C(t) depends only on the immediate past value, C(t-1), and a random shock. Such a model is called a first-order, autoregressive, stochastic process.

A preliminary discussion of the lognormal distribution and auto/correlation functions will simplify presentation of the stochastic model.

The lognormal distribution, LN(m, σ), with median, m, and shape parameter, σ, has a distribution function given by

$$LN(c;m,\sigma) = \int_0^c \frac{1}{\sigma y\sqrt{2\pi}} \exp\{-\tfrac{1}{2}\,[\ln\{(\tfrac{y}{m})^{1/\sigma}\}]^2\}dy \qquad (1)$$

Decreasing values of m cause the probability distribution to concentrate near zero while increasing values spread (instead of shift) probability toward higher values. Decreasing values of σ cause the probability distribution to concentrate about the median while increasing values spread the probability asymmetrically about the median with increasing skewness toward higher values and increasing pile-up near zero.

The mean and variance of the lognormal distribution are a function of both m and σ:

$$\text{mean } LN(m,\sigma) = me^{\frac{1}{2}\sigma^2} \qquad (2)$$

$$\text{variance } LN(m,\sigma) = m^2e^{\sigma^2}(e^{\sigma^2}-1) \qquad (3)$$

The mean is always larger than the median because the distribution is skewed toward the right and the difference between the mean and median increases with σ. The variance of the lognormal distribution increases with both the median and shape parameter.

The natural logarithm of a lognormal random variable, with median m and shape parameter σ, has a normal distribution with mean ln m (natural logarithm of m) and standard deviation σ, i.e., if C ~ LN(m, σ) then ln C ~ N(ln m, σ). This property allows the parameters of the lognormal to be estimated from data using standard statistics for the mean and standard deviation. The result is that the median of the lognormal distribution is estimated by the geometric mean of the data and the shape parameter is estimated by the standard deviation of the logarithms of the data.

Larsen (1971) defined the standard geometric deviation as the quantity $s = e^{\sigma}$. Probabilities from the lognormal distribution, LN(m, σ), are related to the standard normal distribution, N(0, 1), by

$$LN(ms^z;m,\sigma) = N(z;0,1) \qquad (4)$$

In particular, 68% of the probability lies between $\frac{m}{s}$ and ms; 95% of the probability lies between $\frac{m}{s^2}$ and ms^2.

The autocovariance function of a stationary stochastic process, {C(t), t = 1, 2, ...}, measures the covariance between occurrences which are h time units apart. For a given lag time, h, it is defined as

$$Cov(h) = E(C(t)-\mu)(C(t+h)-\mu) \tag{5}$$

where $\mu = EC(t)$ is the mean value of the stochastic process. The autocorrelation function at lag h, is the covariance function at lag h, normalized by the variance of the process, i.e.,

$$\rho(h) = Cov(h)/Cov(0) \tag{6}$$

Autocorrelation functions of natural pollutant time series are characterized by high correlations for small lag times and decreasing dependence with larger lag times. Certain periodic human activities cause spikes at daily and weekly lag times.

A stochastic model which satisfies our four conditions (lognormality-stationarity - autoregressive - realism) can be expressed in terms of the two parameters of the lognormal distribution, m and σ, and a third parameter, λ, called the autocorrelation parameter. The concentration at time t is given in terms of the concentration at time t-1 by

$$C(t) = m\left[\frac{C(t-1)}{m}\right]^{\lambda} Z(t) \quad (|\lambda|<1), \quad t=1,2... \tag{7}$$

In this model Z(t), t = 1, 2, $\cdots$ are independent, lognormally distributed random variables with median equal to one and shape parameter equal to $\sigma\sqrt{1-\lambda^2}$, i.e.,

$$Z(t) \sim LN(1, \sigma\sqrt{1-\lambda^2}) \tag{7a}$$

The parameter, λ, determines the degree of dependence of C(t) on previous concentrations C(t-1), C(t-2), ···. The autocorrelation function of this stochastic process at lag h is given by

$$\rho(h) = (e^{\sigma^2 \lambda^h} - 1)/(e^{\sigma^2} - 1) \quad h>0, \quad |\lambda|<1 \tag{8}$$

This autocorrelation function is a decreasing function of lag time and for appropriate choices of λ and σ it approximates the sample autocorrelation functions found by Pollack (1973) and Barlow and Singpurwalla (1974). When the autocorrelation parameter, λ, equals zero, the autocorrelation function is always zero and the process is completely random with respect to time. When $\lambda = 1$ the autocorrelation function is always one, the variables Z(t) become one (see eq. 7a), and the process is completely determined in time.

As long as $|\lambda|<1$, the concentrations generated by equation (7) will be lognormally distributed with median, m, and shape parameter σ.

A convenient method of generating exposure schedules is obtained by taking logarithms of equation (7); i.e.,

$$\ln C(t) = \ln m + \lambda(\ln C(t-1) - \ln m) + \ln Z(t) \tag{9}$$

Since ln Z(t) is normally distributed with mean zero and standard deviation $\sigma\sqrt{1-\lambda^2}$ one can first generate the logarithm of the stochastic process, using a random normal deviate generator, and then exponentiate the result. To start the recursion, generate ln C(0) from a normal distribution with mean ln m and standard deviation σ.

Stochastic models for exposure schedules introduce another dimension of replication into experimental designs. Any given stochastic treatment schedule is only one of an infinite number of time series which have the same statistics. Referring to the model defined in equation (7) a given treatment is specified by the parameters m, σ, and λ. Equation (7) can be used to generate many time series which provide different schedules for replicate treatments. If plants were equally sensitive to an air pollutant at all times within a growing season then the average growth response to the different replicate time series would be the same. In this case, the relevant estimation problem is to experimentally vary the parameters m, σ, and λ and describe the variation about a growth-response model. If plant sensitivity varies greatly over time, then the paramters, m, σ, and λ might not correlate well with plant growth and some other statistic of the time series, such as the mean of a weighted average of plant sensitivity and the time series, might be appropriate.

It is possible to work with a single replicate time series and vary the median but not alter the shape parameter or the autocorrelation function.

The procedure is to generate a time series from equation (7) using $m = 1$ and then multiply this series by any value of m. The resulting series will have a median, m, but the standard geometric deviation and correlation function will not change. If several exposure schedules are generated in this manner, using different medians, then the peaks and valleys in the different schedules will correspond in time.

Concentrations less than the median occur half of the time and concentrations higher than the median occur half the time, but the frequency at which low and high concentrations occur is determined by the shape parameter, σ. Varying the median concentration corresponds to varying the source strength of a diffuse source, while varying the shape parameter corresponds to varying meteorological conditions. Monitoring data taken from widely separated locations show surprisingly small variation in the shape parameter (Larsen, 1971). However, small variations in σ could be extremely important to plants because of its effect on the frequency of high concentrations.

Varying the correlation parameter, λ, changes the time behavior of the process. With a small value of λ a strip chart of concentration vs. time would look like a comb, while a large value of λ would cause the strip chart to look more like hills and valleys. Two conflicting hypotheses about the affect of λ on plant growth seem reasonable: 1) a highly correlated (λ near 1) concentration regime would reduce growth more than an uncorrelated regime (λ near 0) because the highly correlated series would have incidences of high concentrations which could last for several time units; 2) a highly correlated series would reduce growth less than an uncorrelated series because plants possess adaptive mechanisms that could operate efficiently if the concentration did not change rapidly.

PERIODIC MODELS

The simplest long-term pollutant schedule is a constant level applied night and day throughout the growing season. Such treatments are used for control purposes to quantify variablity within and between experimental chambers.

At the next level of complexity are the exposure schedules of Figure 1. The daily, on-off levels of these schedules are similar to those seen in conventional chronic exposure studies and provide a calibration of our own experimental system with previous studies. The constant levels are set to occur during morning hours, when higher SO_2 levels are usually observed.

A further increase in realism is taken with the schedule seen in Figure 2. As we indicated earlier, the shape of regular fluctuations in pollutant strength depends upon human activity patterns and local meteorological conditions. In the case of SO_2, however, some generalization is possible. A few available studies of diurnal patterns in SO_2 show that urban areas tend to have a bimodal daytime concentration curve, with peaks at midmorning and late afternoon, followed by low, constant nighttime levels (Holzworth, 1973; Munn and Katz, 1959; and Lee et al., 1975).

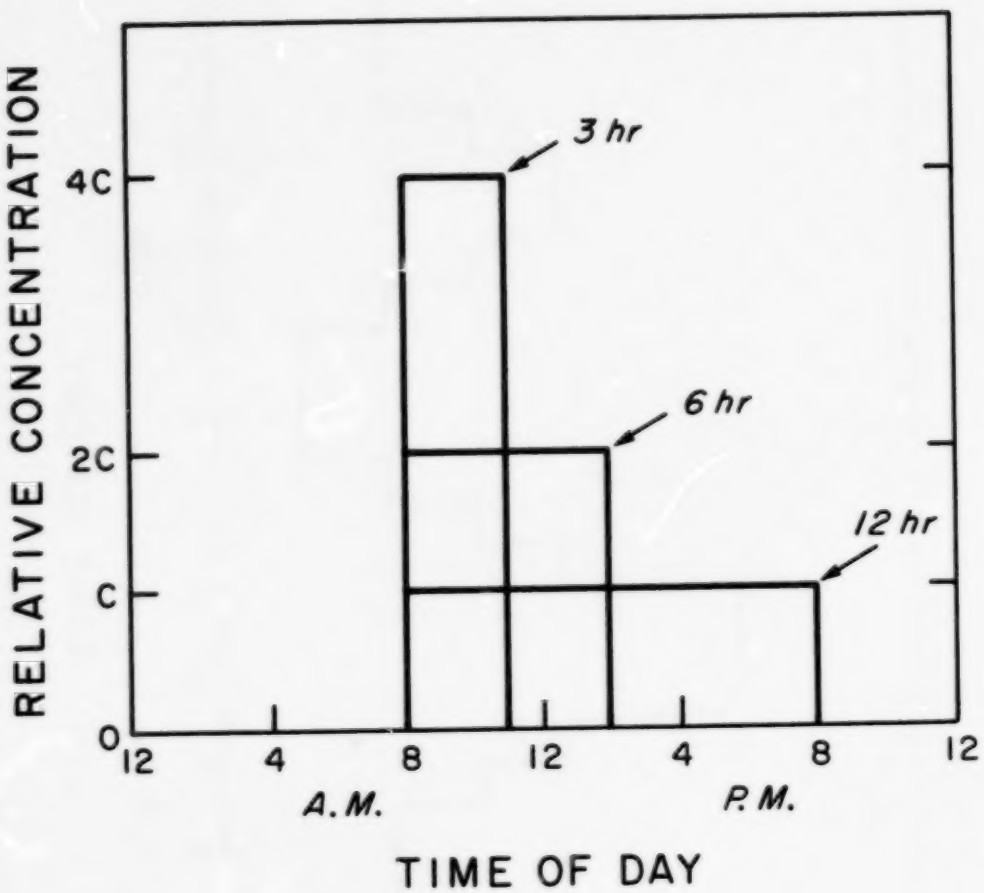

Figure 1. Daily treatment schedules for SO_2 -- applied continuously throughout growing season.

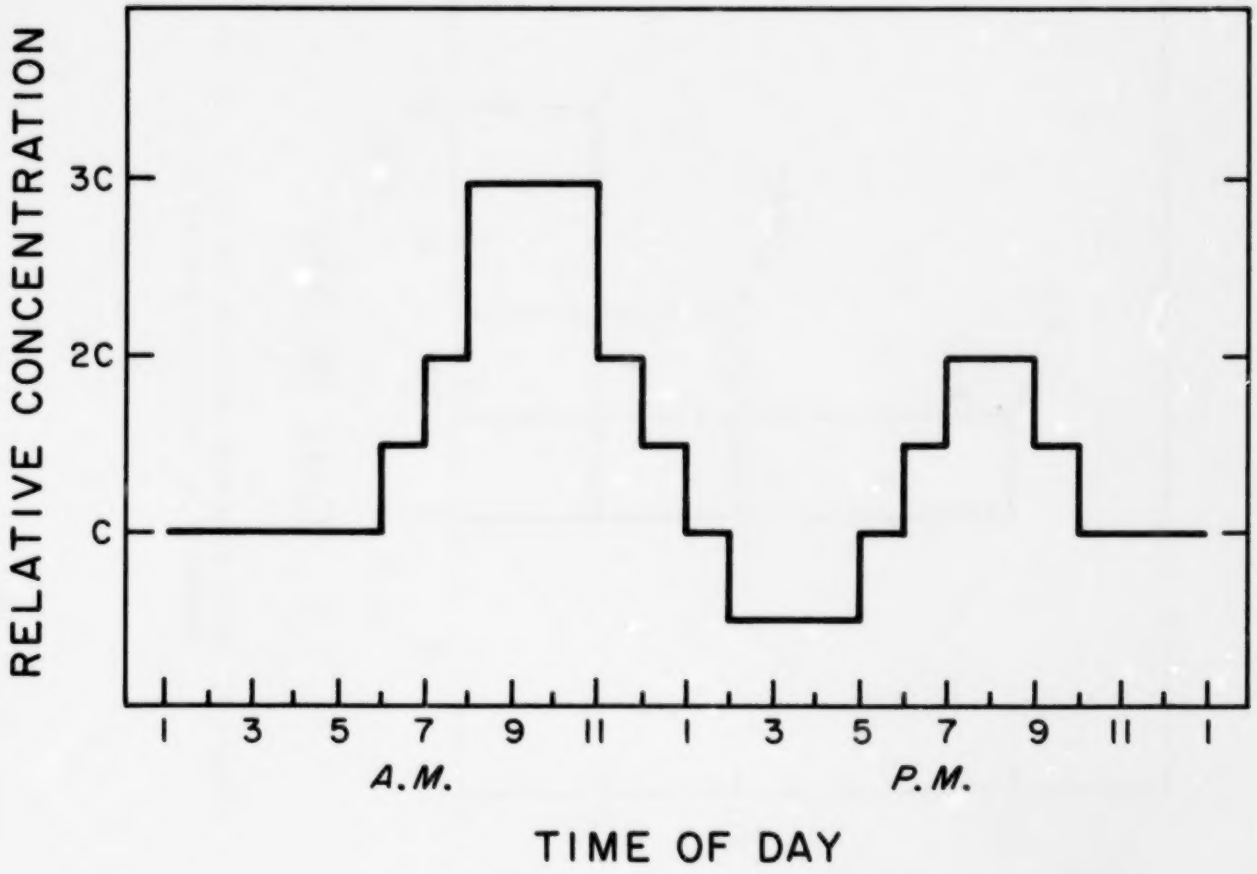

Figure 2. Periodic SO_2 treatment schedule -- applied continuously during growing season.

This pattern is the basis for Figure 2. Plant responses to schedules in Figures 1 and 2 can be compared on the basis of total dose received.

It is possible that plants exposed to the schedules of Figures 1 and 2 may become adapted to the regular fluctuations. In the real world, however, air pollutants are not so predictable, and hour-to-hour changes in concentration appear more random than periodic. It is important, therefore, to determine whether random shocks of pollutant stress reduce growth to a different extent than do predictable stresses. The next model superimposes stochastic fluctuations on periodic patterns such as the one in Figure 2. In this model we assume that the concentration at hour i, i = 1, 2, ..., 24 of any day is a lognormally distributed random variable. Now let Figure 2 be a graph of the median concentrations, m, for every hour of the day. Also assume that all hourly distributions have the same shape parameter, σ. Then a time series of hourly concentrations is generated for hour i of each day by choosing a random sample from a distribution which is LN(m(i), σ). Figure 3 shows a typical sample time series generated by this method. Bimodal daily peaks can be discerned in the figure, following the pattern of Figure 2. Monte Carlo studies with this model have shown that the empirical distribution function for all the hourly levels taken together is well fit by a lognormal curve.

The time series in Figure 3 can thus be summarized statistically by a median and shape parameter, permitting comparison of treatment responses with those obtained from the stationary model, equation (7). Exposure responses can also be compared with those obtained from the purely deterministic treatments of Figures 1 and 2 on the basis of total dose or, in the case of Figure 2, on the basis of median concentration.

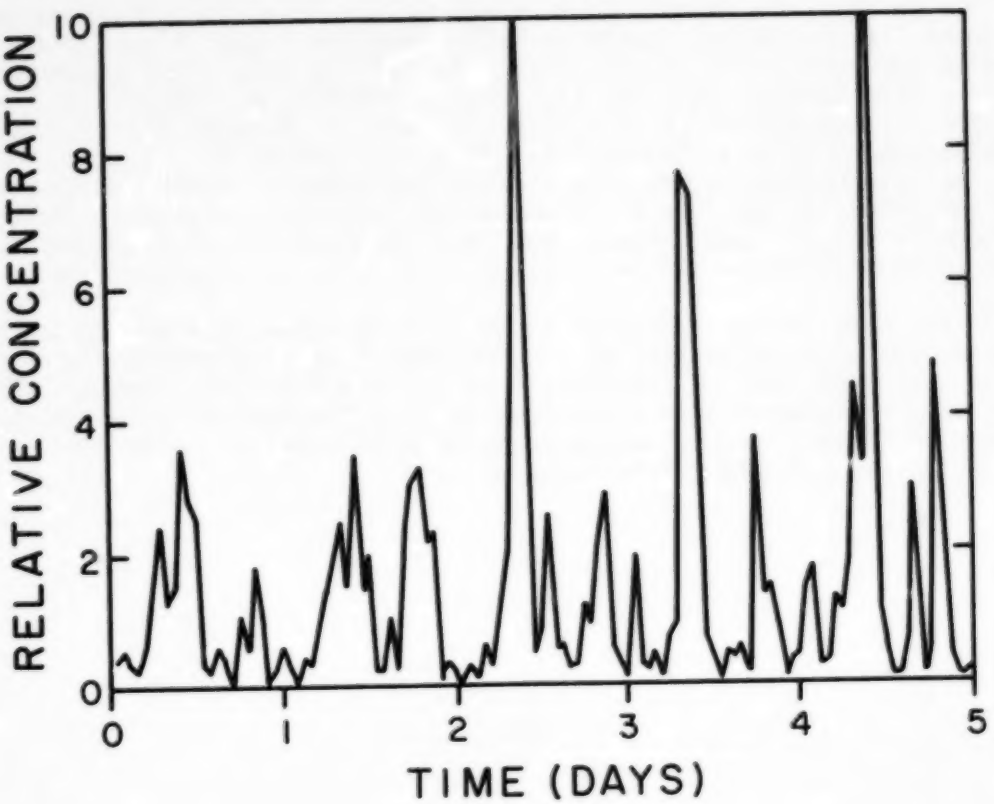

Figure 3. Five-day sample from concentration time series. Series generated by stochastic process with diurnal periodicity in hourly geometric mean concentration.

SECTION 4

DISCUSSION

The stochastic models developed here are good descriptors of natural concentration time series from diffuse sources, such as urban locations. It is not clear that the models are useful in simulating levels from a single point source such as a power plant in rural areas. There are few long-term studies of time series from a point source. Gifford (1974) has suggested, on empirical grounds, that a negative exponential provides the best fit to point source data and Knox and Pollack (1974) argue theoretically that the distribution is Chi Square with two degrees of freedom. The most probable concentration near a point source is zero, and high levels of pollutant are rare and unpredictable.

Exposure schedules which simulate a point source raise problems of replication and prediction of response. Imagine a concentration time series, the length of a growing season, which is dominated by zero levels and has only two or three concentration spikes high enough to affect plant growth. The problem is that the plant growth response to such a schedule may vary widely, depending on the timing of the spikes relative to each other and relative to the developmental stages of the plant.

A realistic appraisal of the effect upon plant growth of an air pollutant may be obtained by exposing plants to simulated ambient fluctuation in pollutant concentration for an entire growing season. A gradient in pollutant source strength, meteorological effects on the time series, and periodic changes in magnitude can be accompiished by varying the parameters of a model. Experiments currently underway are designed to test the sensitivity of plant growth to both probabilistic and deterministic variations in concentration time series. If plant growth does correlate well with parameters of concentration frequency distributions, then the output of regional air pollution models can be applied immediately as input to plant response models.

In summary, stochastic experiments provide a viable alternative to long-term fixed concentration experiments for predicting crop losses caused by SO_2 air pollution. The probabilistic nature of SO_2 time series are fairly well understood and a model which will reasonably simulate realistic exposures has been suggested. Parameters of this model can be varied in field growth chambers to establish their correlation with crop yield. By designing the experiment so that a large number of different time series from the same model are tested then relatively precise probabilistic predictions of crop losses are possible.

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